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Mixing-Controlled Exothermic Fields in Explosions

A. L. Kuhl¹, A. K. Oppenheim² & R. E. Ferguson³

A theoretical model of combustion in explosions at large Reynolds, Peclet and Damköhler numbers is described. A key feature of the model is that combustion is treated as material transformations in the Le Chatelier state plane, rather than "heat release". In the limit considered here, combustion is concentrated on thin exothermic sheets (boundaries between fuel and oxidizer). The products seem to expand along the sheet, thereby inducing vorticity on either side of the sheet that continues to feed the process. The results illustrate the linking between turbulence (vorticity) and exothermicity (dilatation) in the limit of fast chemistry—thereby demonstrating the controlling role that fluid dynamics plays in such problems.

Formulation

Considered here are mixing-controlled exothermic fields in explosions—as typified by combustion of TNT explosion products with air. The TNT-air interface is unstable, and rapidly evolves into a turbulent mixing layer. Combustion takes place in the turbulent velocity field of the hot combustion products, so that the oxidation rate is, in effect, controlled by the turbulent mixing rate. The model recognizes three fluids: *fuel-F* (expanded TNT detonation products), *oxidizer-A* (air), and combustion *products-P*. We consider the exothermic-flow limit—where all molecular transport phenomena associated with viscosity, diffusion, conduction and finite reaction rates are negligible. Hence, the Reynolds number $Re \gg 1$; the Peclet number $Pe \gg 1$; the Damköhler number $Da \gg 1$; and the Mach number: $Ma > 0$. As is typical of combustion in unmixed systems, the fuel reacts with the oxidizer in stoichiometric proportions.

Conservation

In the limit of $Re \gg 1$, the *mixture, m*, obeys the gas dynamic conservation laws :

$$\textbf{Mass:} \quad \partial_t \rho_m + \nabla \cdot (\rho_m \mathbf{u}) = 0 \quad (1)$$

$$\textbf{Momentum:} \quad \partial_t \rho_m \mathbf{u} + \nabla \cdot (\rho_m \mathbf{u} \mathbf{u}) = - \nabla p_m \quad (2)$$

$$\textbf{Energy:} \quad \partial_t \rho_m (u_m + \mathbf{u} \cdot \mathbf{u} / 2) + \nabla \cdot (\rho_m (u_m + \mathbf{u} \cdot \mathbf{u} / 2) \mathbf{u}) = - \nabla \cdot (p_m \mathbf{u}) \quad (3)$$

where ρ, u, p and \mathbf{u} denote the density, specific internal energy, pressure and velocity, respectively. These are supplemented by auxiliary balance laws for mass and energy to follow the evolution of the thermodynamic variables of each fluid throughout the domain. In the limit $Pe \gg 1$, the mass balance equations for the fluids acquire the form:

$$\textbf{Fuel:} \quad \partial_t \rho_F + \nabla \cdot (\rho_F \mathbf{u}) = -\dot{\rho}_s \quad (4)$$

$$\textbf{Air:} \quad \partial_t \rho_A + \nabla \cdot (\rho_A \mathbf{u}) = -\sigma \dot{\rho}_s \quad (5)$$

$$\textbf{Products:} \quad \partial_t \rho_P + \nabla \cdot (\rho_P \mathbf{u}) = (1 + \sigma) \dot{\rho}_s \quad (6)$$

where σ denotes the stoichiometric coefficient ($\sigma = 3.2$ for TNT-air). These equations contain source/sink terms that sum to zero, thereby reproducing the mass conservation relation (1) for the mixture. In the limit $Pe \gg 1$, the energy balance equations for the fluids become:

$$\textbf{Fuel:} \quad \partial_t \rho_F u_F + \nabla \cdot (\rho_F u_F \mathbf{u}) = -p_F \nabla \cdot \mathbf{u} - u_F \dot{\rho}_s \quad (7)$$

$$\textbf{Air:} \quad \partial_t \rho_A u_A + \nabla \cdot (\rho_A u_A \mathbf{u}) = -p_A \nabla \cdot \mathbf{u} - u_A \sigma \dot{\rho}_s \quad (8)$$

$$\textbf{Products:} \quad \partial_t \rho_P u_P + \nabla \cdot (\rho_P u_P \mathbf{u}) = -p_P \nabla \cdot \mathbf{u} + u_P (1 + \sigma) \dot{\rho}_s \quad (9)$$

These equations contain source/sink terms that sum to zero, consistent with the energy conservation (3) for the mixture. Combustion influences these fields through the source $\dot{\rho}_s$.

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Source

Combustion occurs at the *exothermic surface*: $\mathbf{x}_s(t)$ — which acts simultaneously as a *sink* for F & A and a *source* for P . In the limit $Da \rightarrow \infty$, the exothermic surface becomes infinitely thin, and may therefore be represented by a Dirac delta function, δ ; its strength satisfies the stoichiometric consumption rule:

$$\dot{\rho}_s(\mathbf{x}, t) = \begin{cases} \rho_F(\mathbf{x}, t)\delta(t - t_s) & (1 - \lambda < 0) \\ \rho_A(\mathbf{x}, t)\delta(t - t_s)/\sigma & (0 < \lambda < 1) \end{cases} \quad (10)$$

where t_s denotes the time when the fluid particle passes through the exothermic surface, while $\lambda(\mathbf{x}, t) = [\text{Air - Fuel ratio}]/\sigma$. The meaning of this delta-function notation is:

$$\dot{\rho}_s dV dt = \begin{cases} m_F / \delta V & (1 - \lambda < 0) \\ m_A / (\sigma \delta V) & (0 < \lambda < 1) \end{cases} \quad (11)$$

Thermodynamic Properties

The thermodynamic properties of the fluids are represented as loci of states in the Le Chatelier diagram of specific internal energy: u_K as a function of the thermodynamic reference parameter: $w_K = p_K v_K$ ($K = F, A, R, \& P$), as depicted in Fig. 1. The air curve, A , is based on Gilmore (1955). The fuel curve, F , is based on CHEETAH calculations for TNT (Fried, 1995). Air and fuel mix to form reactants R according to the stoichiometric rule:

$$u_R = (u_F + \sigma u_A)/(1 + \sigma) \quad \& \quad w_R = (w_F + \sigma w_A)/(1 + \sigma) \quad (12)$$

Starting with points on R the STANJAN code was used to calculate corresponding thermodynamic equilibrium points on the products curve P . In particular, point i on R transforms to point hp on P for combustion at constant enthalpy & pressure, or to point uv on P for combustion at constant energy & volume. These curves were fit with linear functions:

$$u_A = -0.31909 + 2.65352 w_A \quad \& \quad u_F = -5.28788 + 4.1405 w_F \quad (13)$$

$$u_R = -1.51278 + 2.98856 w_R \quad \& \quad u_P = -4.82385 + 5.40184 w_P \quad (14)$$

where $[u], [w] = \text{kJ/g}$. The above suggest the following form for the equations of state (EOS):

$$e_K = u_K - q_K = F_K(w_K) - C_K w_K \quad (15)$$

Function F_K represents the general curve $e_K = F_K(w_K)$ of Fig. 1; it is well approximated by the linear relation: $F_K(w_K) = C_K w_K$ in the domain of interest (i.e., between points i & f). Its inverse: $F_K^{-1}(e_K) = w_K$ allows one to evaluate w_K from its specific internal energy e_K . Thus, the pressure, and temperature in a pure fluid K may be calculated from

$$p_K = \rho_K w_K = \rho_K F_K^{-1}(e_K) = \rho_K e_K / C_K \quad \& \quad T_K = w_K / R_K = e_K / R_K C_K \quad (16)$$

while for a multi-fluid cell, $K=m$, and the mixture properties are determined from:

$$\rho_m = \sum_K \rho_K \quad e_m = \sum_K \rho_K e_K / \rho_m, \quad C_m = \sum_K \rho_K C_K w_K / \rho_m w_m, \quad R_m = \sum_K \rho_K R_K / \rho_m \quad (17)$$

Combustion

The exothermic source was formulated to model combustion in an adiabatic enclosure. It consisted of three sub-grid processes during the time step: (i) *reactants formation*: fuel and air molecularly mix in stoichiometric proportions, thereby forming reactants according to (12); (ii) *material transformation in the Le Chatelier plane*: reactants are transformed into products according to an *iso-energy* ($u_p = u_R$), *isochoric* ($v_p = v_R$) process—as indicated by the chain-dashed lines of Fig. 1; (iii) *thermal equilibration*: between the post-combustion fluids in the cell.

Application

The model was used to simulate the explosion of a 0.875-kg cylindrical TNT charge in a 16.6- m^3 chamber. The gas dynamic conservation equations for the mixture (1)-(3) were

integrated by means of a higher-order Godunov scheme (Colella & Glaz, 1985), while the auxiliary mass and energy balance equations (4)-(9) of the fluids were advanced as convection equations based on the same scheme. Adaptive Mesh Refinement (Berger & Colella, 1989) was used to follow the details of the mixing structures on the computational grid.

Results

A cross-sectional view of the flow field at 2 *ms* and 5 *ms* is presented in Fig. 2. Material fields are visualized as *yellow* fuel, *blue* air and *red* combustion products. Velocity fields are visualized by means of vorticity contours (*turquoise*=positive & *chartreuse*=negative) and dilatation contours (*black*=negative). Exothermic cells are marked by *white* stars. Expansion of the TNT products drives a cylindrical blast wave that reflects off the side wall ($r = 117\text{cm}$), and then the end wall ($z = 193\text{cm}$). Fuel consumption takes more than 20 *ms*.

Blowups of the flow fields are shown in Fig. 3. They focus on one of the large-scale structures near the chamber wall. The exothermic surface is found on the boundary between the *orange* (fuel-rich) products and the *blue* air. Close inspection reveals that the exothermic surface seems to be sandwiched between vortex sheets of opposite sign. This gives the impression that the products expand preferentially along the exothermic surface rather than normal to it (as in a flame), thereby inducing vorticity on both sides of the surface—forming, in effect, an ***exothermic doublet sheet***. This impression is confirmed by plots of positive dilatation contours (not shown). These vortex sheets supply the surface with fuel from one side and oxidizer from the other via local entrainment—thereby enhancing the burning rate. By 5 *ms*, large-scale structures have caused air to be entrained deep within the mixing layer—resulting in numerous folds in the exothermic surface—leading to a more distributed mode of combustion. Weak (acoustic) shock waves (*black* contours) continually wash over the structures.

Conclusions

According to the present Model, combustion consists of material transformations in the Le Chatelier state plane—thereby rendering the concept of "heat release" as outdated. In fact, heat is not released; rather one transforms from reactants to products without any energy change in the system. In the results presented here for combustion in an isolated chamber (devoid of heat losses or work), this is accomplished as a constant energy process. The condition $u_p = u_R$ then has the effect of eliminating any sources in the mixture energy equation (3), thereby rendering the mixture total energy into a scalar conserved quantity. This is a consequence of representing the thermodynamic properties of the fluids in a self-consistent energy basis in the Le Chatelier plane. Other models are based on relative energy, e ; combustion then corresponds to a heat release in the mixture energy equation:

$$\partial_t \rho_m (e_m + \mathbf{u} \cdot \mathbf{u} / 2) + \rho_m (e_m + \mathbf{u} \cdot \mathbf{u} / 2) \mathbf{u} = - (p_m \mathbf{u}) + Q(1 + \sigma) \dot{\rho}_s \quad (18)$$

where $Q = q_p - q_R$. The present Model avoids such misperceptions.

Numerical simulations based on this Model reveal the characteristics of non-premixed combustion in confined explosions at very large Reynolds numbers. In this case, exothermic fields are controlled by turbulent mixing rather than molecular diffusion. Close examination of the flow field suggests (albeit does not prove) that combustion occurs in an ***exothermic doublet sheet***. The Model presented here illustrates the link between turbulence (=vorticity) and exothermicity (=dilatation) in the limit of fast chemistry ($Da \rightarrow \infty$)—thereby demonstrating the controlling role that fluid dynamics plays in such problems. A companion paper^{*} provides a thermodynamic analysis of this problem.

^{*} A. K. Oppenheim, T-H. Sum & A. L. Kuhl, "Inverse Problem in Explosion and Combustion", 18th ICDERS

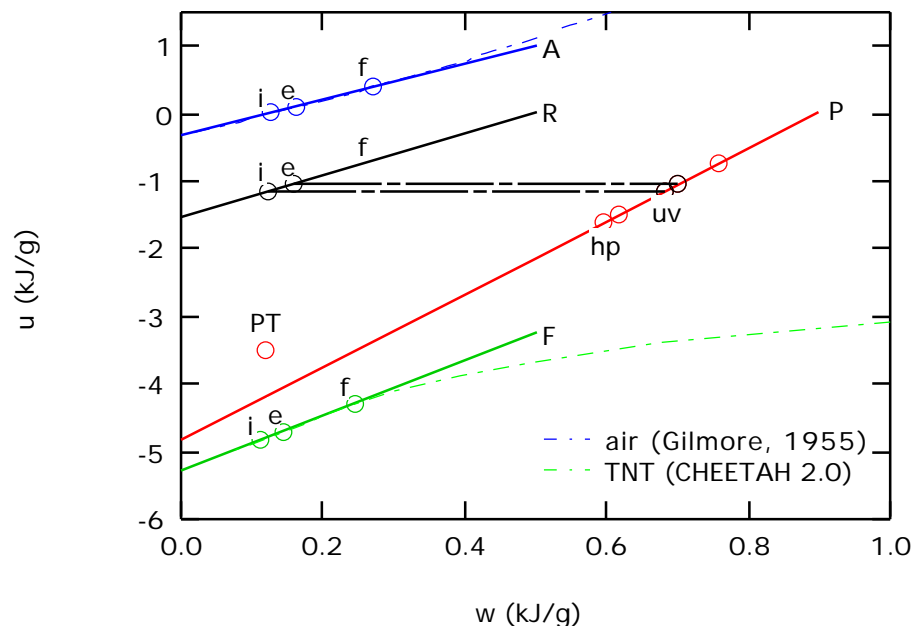


Figure 1. Le Chatelier diagram of states for combustion of Fuel-F (expanded TNT detonation products) with Air-A, forming stoichiometric Reactants-R, which transform into equilibrium combustion products-P.

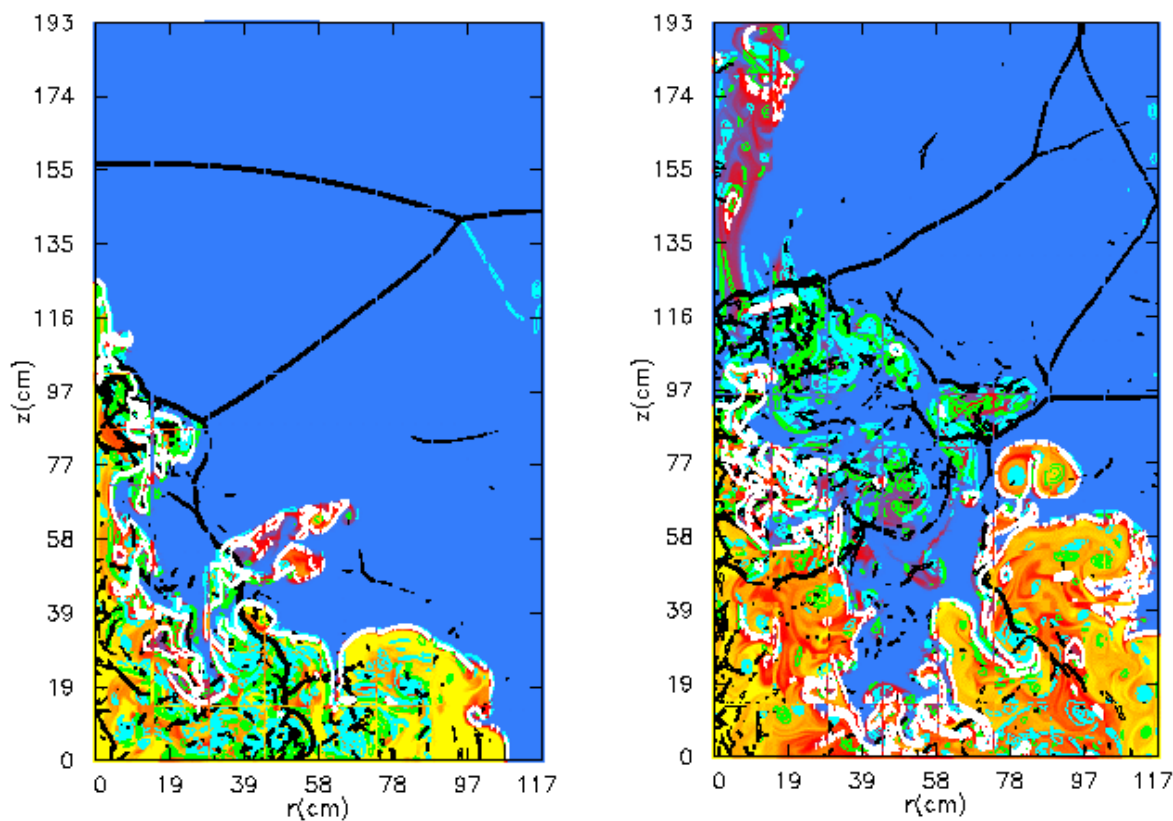


Figure 2. Overall view of the flow field at 2ms and 5ms (for notation, see caption of Fig. 3).

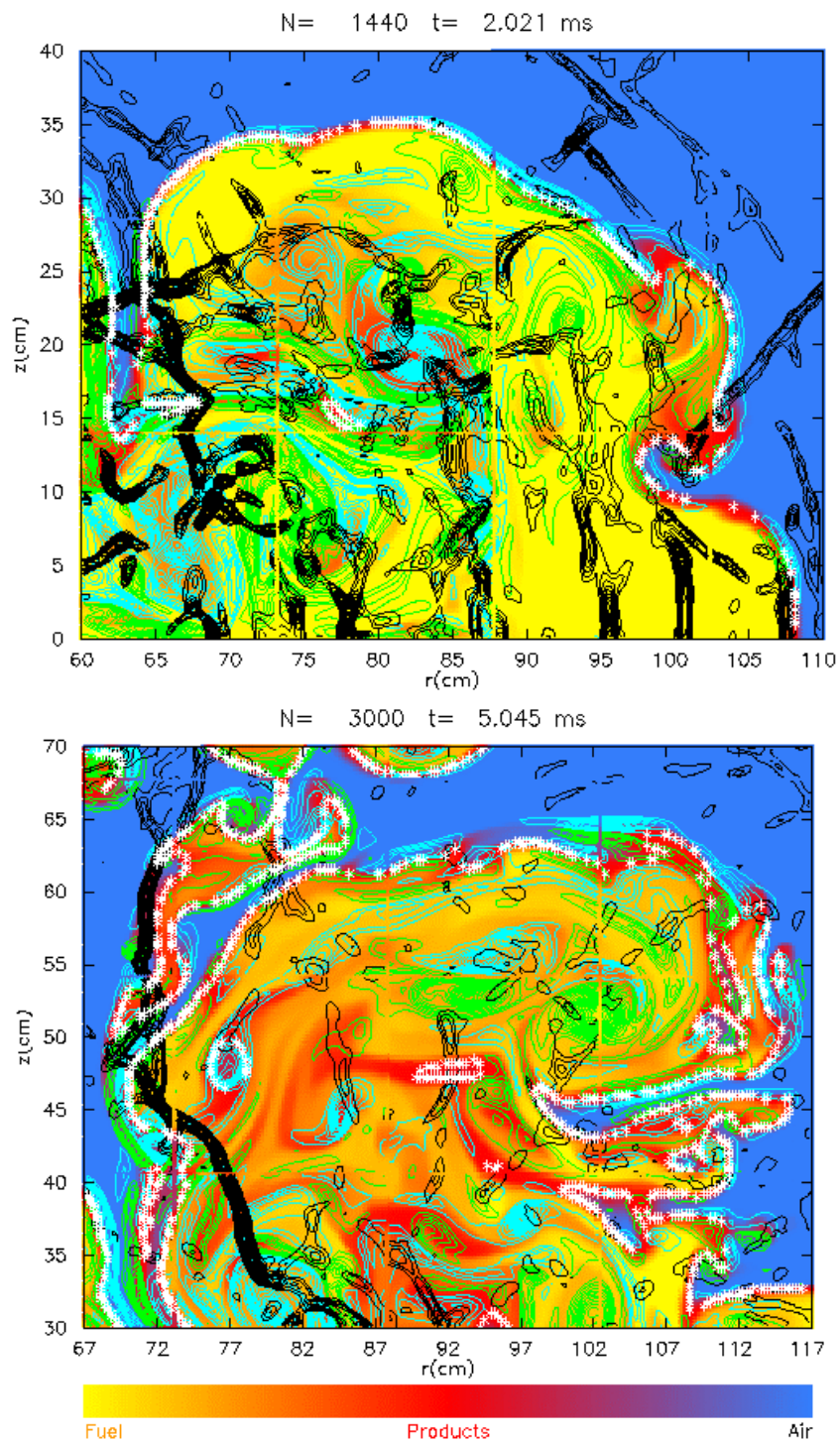


Figure 3. Blow-ups of the flow field created by the explosion of a 1-kg TNT cylinder in a 16.6-m³ chamber at 2 ms and 5 ms. TNT products (shown in yellow) mix with air (depicted as blue) forming combustion products (represented as red). Exothermic cells are marked by white stars. Vorticity contours are turquoise (positive) & chartreuse (negative), while negative dilatation contours are black.